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Dispersion Interactions in Molecular Assemblies from First-Principles Calculations YAN LI, DEYU LU, HUY VIET NGUYEN, GIULIA GALLI, Department of Chemistry and Department of Physics, University of California, Davis, CA, 95616 — We have investigated inter-molecular interactions in weakly bonded molecular assemblies from first principles, by combining exact exchange energies (EXX) with correlation energies defined by the adiabatic connection fluctuation-dissipation theorem, within the random phase approximation (RPA)[1,2]. We present results for three different types of molecular systems: the benzene crystal, the methane crystal and self-assembled monolayers of phenylenediisocyanide. We describe in detail how computed equilibrium lattice constants and cohesive energies may be affected by input ground state wave functions and orbital energies, by the geometries of the molecular monomers in the assemblies, and by the inclusion of zero point energy contribution to the total energy. We find that the EXX/RPA perturbative approach provides an overall satisfactory, first principle description of dispersion forces, in good agreement with experiments and advanced quantum chemistry results. However, binding energies tend to be underestimated and possible reasons for this discrepancy are discussed. This work was funded by DOE/BES DE-FG02-06ER46262 and DOE/SciDAC DE-FC02-06ER25794.[1] Y. Li, D. Lu, H-V. Nguyen and G. Galli, J. Phys. Chem.(submitted). [2]D. Lu, Y. Li, D. Rocca and G. Galli, Phys. Rev. Lett. 102, 206411(2009).

Yan Li

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